Table 1 Data collection and refinement statistics for four CDK2-inhibitor complexes

Data collection	**56**	**22**	**43**	**27**
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
Cell dimensions / Å				
a	52.9	52.8	52.5	53.4
b	70.9	71.0	70.3	72.3
c	72.3	71.8	71.9	72.4
Maximal resolution / Å	1.90	1.30	2.00	2.10
Observations	66017	535908	35160	NA[d]
Unique reflections	23878	63538	15679	14443
Completeness / %	93.3	96.3	85.9	90.1
R_{merge}[a]	0.064	0.046	0.090	NA
Mean I/σ(I)	8.4	20.2	6.8	10.1
Highest resolution bin / Å	1.96-1.90	1.36-1.30	2.07-2.00	2.20-2.10
Completeness / %	85.0	97.2	83.1	NA
R_{merge}[a]	0.28	0.47	0.44	NA
Mean I/σ(I)	1.4	1.8	1.7	1.9

Table 1 cont. Data collection and refinement statistics for four CDK2-inhibitor complexes

Refinement	**56**	**22**	**43**	**27**
Protein atoms (chain A)	2311	2372	2371	2297
Inhibitor atoms (chain B)	18	17	18	18
Waters (chain W)	310	344	186	133
Resolution range (Å)	50-1.90	50-1.30	50-2.00	20-2.10
R_{conv} [b] (%)	15.4	16.3	19.4	21.4
R_{free} [c] (%)	23.4	19.9	26.0	28.7
Mean protein temperature factor (Å^2)	21.6	19.9	23.9	29.8
Mean ligand temperature factor (Å^2)	24.7	23.8	32.7	35.1
Mean solvent temperature factor (Å^2)	34.2	34.0	31.2	36.9

[a] $R_{merge} = \Sigma_h\Sigma_j |I_{h,j} - \bar{I}_h|/\Sigma_h\Sigma_j|I_{h,j}|$, where $I_{h,j}$ is the jth observation of reflection h.
[b] $R_{conv} = \Sigma_h||F_{oh}| - |F_{ch}||/\Sigma_h|F_{oh}|$, where F_{oh} and F_{ch} are the observed and calculated structure factor amplitudes respectively for the reflection h.
[c] R_{free} is equivalent to R_{conv} for a 5% subset of reflections not used in the refinement.
[d] NA – data not available.